

# A FORMULATION OF FULLY COUPLED THERMAL–HYDRAULIC–MECHANICAL BEHAVIOUR OF SATURATED POROUS MEDIA—NUMERICAL APPROACH

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## SUMMARY

The theoretical aspects of fully coupled thermohydromechanical behaviour of saturated porous media are presented. The non-linear behaviour of soil skeleton is assumed. A new concept called 'thermal void ratio state surface' is introduced to include thermal effects, and the stress state level influence on volume changes. The fluid phase flows according to Darcy's law and energy transport is assumed to follow Fourier's law classically. Variation of water permeability, water and solid unit weight due to thermal effects and pore pressure changes are included. A finite element package is developed based on final matrix form obtained from discretization of integral form of field equations by finite element method and integration in time. A very good agreement between the theoretical predictions and the experimental results was obtained for the several simple problems proposed by other authors. © 1997 by John Wiley & Sons, Ltd.

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## 1. INTRODUCTION

A great deal of attention is focused on coupled thermohydromechanical behaviour of fluid-saturated porous media in diverse areas such as: extraction of oil or geothermal energy, road subgrade and pavement subjected to heating–cooling cycles, frictional heating in fault zones in rocks and soils and specially high-level radioactive waste disposal.

Detailed and deep knowledge of hydromechanical, hydrothermal and thermomechanical processes and their interdependence is necessary for describing a fully coupled behaviour of fluid saturated media in the presence of heat flow. Different aspects and issues of thermal behaviour of soils can be considered. In this study, the chain of events caused by nuclear waste disposal is of prime concern.

The interaction of heat sources (canisters and containers of radioactive waste materials) and surrounding repository solids (near field) including hydrothermomechanical coupling phenomena in soil are investigated. In the waste disposal multi-barrier design, the canister and metal containers form the first barrier, where as the surrounding repository soils or rocks form a long-term barrier against contamination. In this context, the hydromechanical response of soil

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and rocks to waste decay heat is affected by temperature change in several ways. Mechanical and hydraulical properties of soils may change during the heating and cooling cycles. Excess pore pressure generation under undrained conditions and deformation of the porous matrix are the important effects of increase in temperature. These main issues will be addressed in this study but the chemical, mineralogical and microstructural changes which could be important and affect the plastic behaviour of soil are neglected here.

Different aspects of these phenomena can be treated by various theories. Pinder<sup>1</sup> and Wang *et al.*<sup>2</sup> have studied in detail the coupled phenomena of heat and fluid flow, known as hydrothermal flow. One of the pioneering study on isothermal hydromechanical coupling is that of Biot's consolidation theory.<sup>3,6</sup> Rice and Cleary<sup>7</sup> have recast this theory by giving the straightforward physical interpretations. The numerical solutions of consolidation theory were developed with the advent of computers.<sup>8,9</sup> The numerical solution of more general theory of consolidation with a more realistic treatment of hydromechanical behaviour of saturated porous media for dynamic and quasi-static loading (marine application) considering the new definition of effective stress for anisotropic and non-linear stress-strain relationship is introduced by Gatmiri.<sup>10-12</sup>

An account of the state of the art on the thermomechanical coupling of continuous or discontinuous media is given by Baca<sup>13</sup> and Tsang.<sup>14</sup> Thermoelasticity in which the effect of temperature changes on mechanical behaviour in linear elasticity is considered, is a well-known theory.<sup>15</sup> From review of models treating the thermohydromechanical behaviour of two-phase porous media, it appears that an important number of models is based on extension of isothermal consolidation theory to account for the effect of thermal expansion of elastic matrix (e.g. References 16-19). In these studies the effect of convection has been disregarded and the effect of thermal expansion and compressibility of pore fluid were neglected. Such an approach can only deal with an indirect coupling between the energy and fluid flow.<sup>20</sup>

Based on the mixture theory (e.g. References 21-23), a quasi-static infinitesimal theory of thermoelastic consolidation was developed by Aboustit *et al.*<sup>24</sup> In this approach the solid is assumed to be elastic linear and saturated by an incompressible fluid. The convection is ignored. The coupling terms between temperature and pressure do not appear in the formulation presented by Aboustit *et al.*<sup>25</sup> This results in a symmetric general matrix.

A numerical approach of hydrothermoelasticity for fractured rock is given by Noorishad *et al.*<sup>20</sup> Booker and Savvidou<sup>26</sup> provided analytical solutions for a thermoelastic consolidation which takes into account the differential thermal expansion of the pore water and soil skeleton. This approach is based on simple concepts of volume constraint and the effective stress principle. The temperature field is uncoupled from pressure and displacements by ignoring the mechanical contributions to energy balance and the convective terms.

An extension of the isothermal theory of Rice and Cleary<sup>7</sup> is given by McTigue<sup>27</sup> by considering the compressibility of fluid and solid constituents, as well as thermal expansion of both phases. This theory has been specialized to the case of one-dimensional deformation, and exact solutions to several problems have been given. This theory is a fully linearized theory, and in addition to many limitations, the convective heat transfer is also neglected. One case of interest has been reported by Lewis *et al.*<sup>28</sup> in which a coupled finite element model for the analysis of the deformation of elastoplastic porous media under the effect of heat and fluid flow is given. The convection terms are neglected in this formulation. In this thermoelastoplastic model, a temperature-independent critical state yield function has been assumed. In two numerical examples, comparisons with results of Aboustit *et al.*<sup>25</sup> and with those of Booker and Savvidou<sup>26</sup> are made.

Britto *et al.*<sup>29</sup> have presented the results of the comparison of centrifuge test data and the finite element analysis based on the formulation presented by Britto in the frame of elastic and elastoplastic behaviour of soil. The elastoplastic model used by Britto *et al.*<sup>29</sup> is an extension of CRISP (Critical State Program) to thermal effect. The yield function is independent of temperature. In this model, modified Cam-Clay elliptical yield surface with an associated flow rule is chosen. For the range of temperature change encountered in nuclear waste disposal in clay, with a very low permeability such as  $10^{-9}$  m/s, the Rayleigh number is very small and heat transfer takes place by pure conduction, while convection heat transfer has unimportant contribution. This study shows that, for the case of canisters buried in an overconsolidated clay, the pore pressure generation is underpredicted grossly. Good agreement was found between the observed and predicted temperatures and pore pressure distribution in normally consolidated soil.

Thermoplasticity of saturated clay has been studied by a U.S.-Italian research group (Duke University and ISMES in Bergamo, Italy). Two natural clays, Boom clay from Belgium and Pasquasia from Italy, and one remolded clay, Pontida silty clay, have been used in their experimental program. These clays are different in their mineral content and activity.<sup>30</sup> A complete set of constitutive equation governing the fully coupled thermoelastoplastic behaviour of a saturated clay is presented.<sup>31</sup> This model takes into account a temperature-dependent yield surface with a non-associated flow rule.

A complete set of governing equations of dynamic isothermal behaviour for a fully saturated porous elastic media based on Biot's<sup>5,6</sup> theory has been given by Gatmiri<sup>10</sup> and extended to anisotropic and non-linear behaviour in quasi-static conditions.<sup>11,12</sup> Non-isothermal behaviour of saturated porous media should be modelled by using the equilibrium equation of solid skeleton together with the continuity equations of heat and fluid flow. In this paper the modifications due to heat flow are introduced to the first author's previous works, and only the case of single fluid phase is considered. The same modifications can be used also for a multiphase flow.

## 2. FIELD EQUATIONS

For an isothermal fully saturated porous media, two field variable quantities related to solid skeleton and fluid phase must be defined. For a non-isothermal case, temperature related to heat flow should be chosen as the third field variable. Two former ones are: the displacement of the solid skeleton  $u_i$  and the average relative displacement of the fluid with respect to solid skeleton  $w_i$ , which is measured in terms of volume of fluid per unit total cross-sectional area of bulk medium. Considering the displacement of the fluid as  $W_i$ , we can write

$$w_i = n(W_i - u_i) \quad (1)$$

where  $n$  is the porosity of the sediment.

### 2.1. Solid skeleton behaviour

Assuming an anisotropic non-linear elastic media in the frame of small deformation, the field equations for isothermal behaviour of solid skeleton can be given as follows:<sup>10-12</sup>

$$\sigma_{ij,j} + \rho g_i = 0 \quad \text{on } D \times (0, \infty) \quad (2)$$

$$\sigma''_{ij} = \sigma_{ij} + A_{ij}p \quad \text{on } D \times (0, \infty) \quad (3)$$

$$\sigma''_{ij} = D_{ijkl}\varepsilon_{kl} \quad D \times (0, \infty) \quad (4)$$

$$\varepsilon_{ij} = (u_{i,j} + u_{j,i})/2 \quad D \times (0, \infty) \quad (5)$$

where equation (3) gives a new definition of effective stress  $\sigma''_{ij}$  in which the components of tensor  $A_{ij}$  are defined by  $\delta_{ij}\beta_{ij}D_{ijkl}\delta_{kl}$  for any pair of indices and  $i \neq j \Rightarrow A_{ij} = 0$ .  $\beta_{ij}$  are six compliance coefficients that are related to the compressibility of grain such as  $\beta_{ij} = \delta_{ij}/3K_s$ . In the above equations,  $\varepsilon_{ij}$  is the strain tensor,  $\sigma_{ij}$  the total stress tensor,  $p$  the pore pressure,  $D_{ijkl}$  the stress-strain relationship tensor,  $u_i$  the vector of displacement of solid skeleton,  $K_s$  the bulk modulus of solid particles,  $\rho$  the density of assembly of solid and fluid (bulk mass density),  $g_i$  the gravity acceleration vector and  $\delta_{ij}$  the Kronecker symbol.

For an isotropic behaviour as a particular case,  $A_{ij}$  can be simplified as  $\alpha = 1 - K'/K_s$  given by Biot<sup>6</sup> where  $K'$  is the effective bulk modulus ( $= (2G + 3\lambda)/3$ ) where  $G$  and  $\lambda$  are Lamé's coefficients) and the effective stress definition given by Terzaghi can be found by introducing  $\alpha = 1$ . The isothermal constitutive equation should be modified for a non-isothermal case by considering the total strain of the skeleton expanded as follows:

$$\sigma''_{ij} = D_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^c - \varepsilon_{kl}^p - \varepsilon_{kl}^t - \varepsilon_{kl}^0) \quad (6)$$

where  $\varepsilon_{kl}$  is the total strain of the skeleton,  $\varepsilon_{kl}^c$  is the creep strain,  $\varepsilon_{kl}^t$  is the thermal strain,  $\varepsilon_{kl}^p$  is the volumetric strain caused by uniform compression by pore water, and  $\varepsilon_{kl}^0$  is all other strain not directly associated with stress changes.

The creep phenomenon is neglected and  $\varepsilon_{kl}^0$  is considered to be equal to zero for further developments. Equilibrium equation and constitutive law for a non-isothermal isotropic and non-linear case can be written as follows:

*Equilibrium equation:*

$$\sigma_{ij,j} + \rho g_i = 0 \quad (7)$$

*Constitutive law under small strain assumption:*

$$\sigma''_{ij} = D_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^p - \varepsilon_{kl}^t) \quad (8)$$

with the definition of effective stress as

$$\sigma''_{ij} = \sigma_{ij} - \alpha p \delta_{ij} - \beta T \delta_{ij} \quad (9)$$

where  $\alpha$  is the Biot hydromechanical coupling coefficient and  $\beta$  is the thermomechanical coupling coefficient ( $= (2G + 3\lambda)\alpha_s = 3K'\alpha_s$ , where  $\alpha_s$  is the solid thermal expansion coefficient.). In this formulation,  $D_{ijkl}$  is a stress and temperature-dependent tensor.

## 2.2. Pore fluid motion equations

Starting with an isothermal anisotropic and non-linear case developed by Gatmiri,<sup>10-12</sup> we can write the following.

*Fluid mass conservation:*

$$-\dot{w}_{i,i} = A_{ij}\dot{\varepsilon}_{ij} + C_{aai}\dot{p} \quad (10)$$

*Water flow equation (Darcy law):*

$$\dot{w}_j = -\Lambda_{ij}(p_{,i} + \rho_w g_i) \quad (11)$$

where  $\Lambda_{ij}$  is the permeability tensor and

$$C_{aai} = n/K_w + (1 - n)/K_s - 3\beta_{ij}^2 D_{ijkl} \delta_{kl} \quad (12)$$

with  $K_w$  being the bulk modulus of pore water. In the development of the above equations, the hydraulic and mechanical anisotropy and compressibility of fluid and solid particles and validity of Darcy's law are assumed.

For an isotropic case, equation (12) becomes  $C_{aa} = n_0/K_w + (1 - n_0)/K_s - K'/K_s^2 = 1/M$ , given by Biot<sup>6</sup> and (Gatmiri<sup>10</sup>), where  $n_0$  is the initial porosity. For a non-isothermal case, the thermal effects on the rate of fluid accumulation in mass conservation equation should be considered. The solid density  $\rho_s$  and the pore water density  $\rho_w$  are assumed to be pressure and temperature dependent:

$$\rho_w = \rho_w(p, T), \quad \rho_s = \rho_s(p, T) \quad (13)$$

the rate of changes of fluid density and solid density under the variation of pressure and temperature can express the contributions in fluid accumulations:

$$\frac{\partial \rho_w}{\partial t} = \left( \frac{\partial \rho_w}{\partial P} \right)_T \frac{\partial p}{\partial t} + \left( \frac{\partial \rho_w}{\partial T} \right)_P \frac{\partial T}{\partial t} \quad (14)$$

$$\frac{\partial \rho_s}{\partial t} = \left( \frac{\partial \rho_s}{\partial P} \right)_T \frac{\partial p}{\partial t} + \left( \frac{\partial \rho_s}{\partial T} \right)_P \frac{\partial T}{\partial t} \quad (15)$$

$(\partial \rho_w / \partial P)_T$  is the variation of fluid density under pressure changes at constant temperature conditions and  $(\partial \rho_w / \partial T)_P$  is the fluid density changes, caused by temperature variation, at constant pressure conditions.

The variation of permeability tensor under thermal effects in flow equation should be taken into account by considering the effect of temperature changes on dynamic viscosity ( $\nu$ ). The effect of pressure changes on dynamic viscosity can be neglected,

$$\nu = \nu(p, T) = \nu(T), \quad \Lambda_{ij} = f(T, e) \quad (16)$$

where  $e$  is the void ratio.

Via the coupling terms defined previously, the change of solid particles size due to variation of stress and temperature have been considered. Finally, after some mathematical manipulations the mass balance equation of pore fluid and Darcy law for non-isothermal case become

$$\dot{\zeta} = -\dot{w}_{i,i} = \alpha \dot{e}_{ii} + C_a \dot{P} + C_h \dot{T} \quad (17)$$

$$\dot{w}_j = -\Lambda_{ij}(p, i + \rho_w g_i) \quad (18)$$

where

$$\Lambda_{ij} = \Lambda_{wij} \left( \frac{v_0}{v} \right) \left( \frac{e}{e_0} \right)^3 \Rightarrow \Lambda_{ij} = f(T, e) \quad (19)$$

$$\rho_w = \rho_w(p, T), \quad \rho_s = \rho_s(p, T), \quad \nu = \nu(p, T) \approx \nu(T). \quad (20)$$

Here  $C_a$  is the mixed fluid–solid compressibility:  $(= (\alpha - n)/K_s + (n/K_w))$ ,  $C_h$  is the coefficient of undrained thermal expansion of the mixture  $(= (\alpha - n)\alpha_s + n\alpha_w)$ , where  $\alpha_s$ , and  $\alpha_w$  are coefficients of thermal expansion of solid and water,  $e_0$  and  $v_0$  are the void ratio and water dynamic viscosity at ambient temperature,  $e$  and  $\nu$  are the void ratio and water dynamic viscosity at a given temperature, and  $\zeta$  is the volumetric fluid content.

### 2.3. Energy transport equations and Fourier law

Assuming the absence of fluid shearing stresses in the macroscopic scale and neglecting the energy associated with the thermal contact equilibrium between solid and fluid, and fluid dilatancy, the energy balance equation can be written. This equation states that the increase of internal energy must be balanced by the rate of inflow into a control volume.<sup>7,33</sup>

*Energy conservation equation:*

$$\rho_w C_w T_{,i} \dot{w}_{i,i} - h_{i,i} = \beta \dot{T}_0 \dot{\epsilon}_{ii} + C_b \dot{T} - C_T T_0 \dot{p} \quad (21)$$

*The Fourier law as an equation governing the heat flow:*

$$h_i = -k_{ij} T_{,j} \quad (22)$$

where  $h_i$  is the heat flow vector,  $k_{ij}$  the solid–fluid mixture thermal conductivity tensor ( $= nk_{ij}^w + (1-n)k_{ij}^s$  with  $k_{ij}^w$  and  $k_{ij}^s$  being the fluid and solid thermal conductivity tensors),  $T_0$  the absolute temperature in the stress-free state,  $C_b = (\rho C)_M - \{(1-n)C_s \rho_s \alpha_s + nC_w \rho_w \alpha_w\} T_0$  where  $(\rho C)_M$  is the solid–fluid mixture heat capacity ( $= (1-n)\rho_s C_s + n\rho_w C_w$ ),  $C_s$  the specific heat capacity of the solid,  $C_w$  the specific heat capacity of the water and  $C_T = (1-n)C_s \rho_s / K_s + nC_w \rho_w / K_w$ .

Through the established equations, a complete set of mathematical formulation of the thermohydromechanical behaviour of a saturated porous medium is given. The general initial and boundary conditions must be associated with the foregoing equations in order to complete the mixed initial boundary value problem of thermohydromechanics. These conditions are the discussed next.

### 2.4. General initial and boundary conditions

$$u(x, 0) = 0 \quad \text{on } \Omega \quad (23)$$

$$p(x, 0) = p_0 \quad \text{on } \Omega \quad (24)$$

$$T(x, 0) = T_0 \quad \text{on } \Omega \quad (25)$$

$$\text{I} \begin{cases} u(x, t) = \bar{u}(x, t) & \text{on } S_1 x[0, \infty) \\ \sigma(x, t) \cdot \underline{n} = \bar{\sigma}(x, t) & \text{on } S_2 x[0, \infty) \end{cases} \quad (26)$$

$$\text{II} \begin{cases} p(x, t) = \bar{p}(x, t) & \text{on } S'_1 x[0, \infty) \\ V_w \cdot \underline{n} = q_w(x, t) & \text{on } S'_2 x[0, \infty) \end{cases} \quad (27)$$

$$\text{III} \begin{cases} T(x, t) = \bar{T}(x, t) & \text{on } S''_1 x[0, \infty) \\ \rho_w C_w V_w^i T \cdot \underline{n} - h_i \cdot \underline{n} = q_t(x, t) & \text{on } S''_2 x[0, \infty) \end{cases} \quad (28)$$

Here  $\Omega$  represents the considered domain and  $S, S', S''$  represent the different parts of the boundary of domain on which the displacement or stress, pressure or fluid flow, and temperature or heat flow are given. The initial conditions for the different variables ( $u, p, T$ ) must be introduced. In geotechnical applications, the initial displacements are seldom introduced however.

### 3. CONSTITUTIVE LAW FOR STRESS-STRAIN-TEMPERATURE

Reconsidering equations (8), the constitutive equation can be written in incremental form

$$d\sigma''_{ij} = D_{ijkl}(d\varepsilon_{kl} - d\varepsilon_{kl}^p - d\varepsilon_{kl}^t) \quad (29)$$

strain increment  $d\varepsilon^t$  due to temperature increment  $dT$  can be written as

$$d\varepsilon^t = D_T^{-1} dT \quad (30)$$

where  ${}^tD_T^{-1} = \beta_i [1 \ 1 \ 0]$  in which  $\beta_i$  is stress and temperature dependent. Substituting equation (30) into equation (29), one can obtain

$$d\sigma'' = D d\varepsilon'' - C dT \quad (31)$$

with  $C = D D_T^{-1}$  and  $d\varepsilon'' = d\varepsilon - d\varepsilon^p$  defined as effective strain. The stress-strain relationship matrix can be presented by

$$D = \frac{3B}{9B - E} \begin{bmatrix} 3B + E & 3B - E & 0 \\ 0 & 3B + E & 0 \\ 0 & 0 & E \end{bmatrix} \quad (32)$$

assuming non-linear stress-strain behaviour, using Kondner-Duncan (hyperbolic) model, isothermal tangent modulus with a hyperbolic variation can be given as

$$E_L = K_L P_{\text{atm}} \left( \frac{\sigma_3}{P_{\text{atm}}} \right)^n (1 - R_f S_r)^2 \quad (\text{loading}) \quad (33)$$

$$E_u = K_u P_{\text{atm}} \left( \frac{\sigma_3}{P_{\text{atm}}} \right)^n \quad (\text{unloading}) \quad (34)$$

with  $S_r$  the stress ratio ( $= (\sigma_1 - \sigma_3)/(\sigma_1 - \sigma_3)_{\text{ult}}$ , where  $\sigma_1, \sigma_3$  are the principal stresses and  $p_{\text{atm}}$  is the atmosphere pressure),  $K_L, K_u$  the modulus number (dimensionless), and  $n$  and  $R_f$  are constants. Considering the effect of the heating, the above equations become

$$E = (E_i + E_t)(1 - R_f S_r)^2 \quad (\text{loading}) \quad (35)$$

$$E = E_i + E_t \quad (\text{unloading}) \quad (36)$$

with

$$E_i = K_L P_{\text{atm}} \left[ \frac{\sigma_3}{P_{\text{atm}}} \right]^n \quad (37)$$

$$E_t = m_1 T \quad (38)$$

In order to calculate the bulk modulus, the volumetric strain can be taken into account via void ratio state surface which depends on the temperature.

It is obvious that in each closed stress-temperature cycle, the energy and thermoelastic strain must be recoverable. Volumetric thermoelastic deformation can be found by deriving from the complementary energy potential using the assumptions of logarithmic stress-strain law and a non-linear-stress-dependent thermal expansion coefficient. The thermoelastic variation of void

ratio can be given by

$$\Delta e = C_{cv} \ln \frac{p'}{p'_g} + (1 + e_0) \alpha(\Delta T, p') \Delta T \quad (39)$$

where

$$\alpha(\Delta T, p') = \alpha_0 + \alpha_2 \Delta T + (\alpha_1 + \alpha_3 \Delta T) \ln \frac{p'}{p'_g} \quad (40)$$

in which  $\alpha_0, \alpha_1, \alpha_2, \alpha_3$  are constants,  $C_{cv}$  is isothermal compressibility index using the coordinates of  $e$  and  $\ln p'$ ,  $p'$  is effective mean stress,  $e_0$  is initial void ratio and  $p'_g$  is the isotropic component of geostatic stress at which the elastic strain is null. Stress at the end of saturation can be taken as  $p'_g$  under laboratory conditions. This equation is given based on the experimental results found in program research carried out in ISMES, Bergamo, Italy; thus the thermal void ratio state surface expression can be given by

$$e = e_0 + C_{cv} \ln \frac{p'}{p'_g} + (1 + e_0) \alpha(\Delta T, p') \Delta T \quad (41)$$

A schematic representation of this surface is shown in Figure 1.

The bulk modulus  $B$  can be defined by

$$d\varepsilon_v = \frac{1}{1 + e_0} \frac{\partial e}{\partial p'} dp' = \frac{1}{B} dp' \quad (42)$$

$$B = (1 + e_0) \frac{p'}{C_{cv} + (1 + e_0)(\alpha_1 + \alpha_3 \Delta T) \Delta T} \quad (43)$$

thus

$$D = D(B, E) = D(\sigma', T) \quad (44)$$

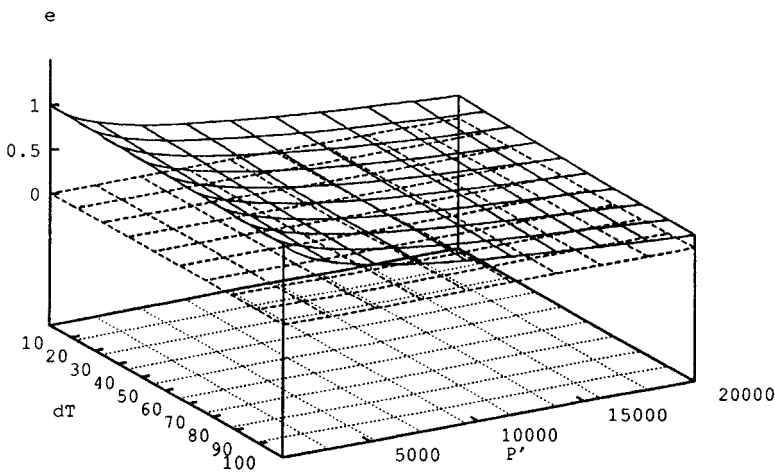


Figure 1. Schematic state surface of thermal void ratio



The thermal effects represented by  $D_T$  can be given by

$$d\varepsilon_T = \frac{I}{I + e_0} \frac{\partial e}{\partial T} dT = \beta_T^i m dT \quad (45)$$

$$\beta_T = \left[ \alpha_0 + 2\alpha_2 \Delta T + (\alpha_1 + 2\alpha_3 \Delta T) \ln \frac{p'}{p_g} \right] \quad (46)$$

As seen in the above new formulation the non-linear stress-dependent thermal expansion coefficient  $\beta_T$  is introduced. The shear strains are assumed to be due to mechanical effects.

As discussed in the previous section, there is no significant effect of temperature change in peak undrained shear strength. But for drained cases, an increase in peak shear strength is observed with temperature increase. Variation of shear strength can be given by

$$\tau_{ult} = C + \sigma'_n \operatorname{tg} \varphi(T) \quad (47)$$

The stress ratio can be presented:

$$S_r = \frac{\sigma'_1 - \sigma'_3}{2\tau_{ult}} \quad (48)$$

the lack of reliable information on the shear strength of soils leads, for instance, to consider an approximate evaluation of shear strength variation under heating based on the suggested formula for the friction angle variation under the temperature change given by Houston *et al.*<sup>33</sup> such as

$$\varphi(T) = \varphi_0 \exp(0.002T) \quad (49)$$

#### 4. SOLUTION APPROACH

The development of analytical solutions for the governing partial differential equations of the thermohydrummechanical behaviour of saturated soils regarding its complexity is very difficult even for the simple conditions and probably impossible for the real and general boundary and initial conditions. The existing analytical solutions are based on the simple assumptions which reduce the usefulness and applicability of the solutions to the practical cases. The known numerical approaches such as finite difference, finite element or boundary element methods can be easily used to find the solutions to the most general boundary and initial conditions. The Bubnov–Galerkin integral forms of field equations has been developed such as a basis of the spatial and temporal discretized matrix form.

##### 4.1. Spatial discretization

Application of weighted residual method and the Galerkin choice of weighted functions to the equations represented in the terms of nodal point values of the field variables for the total spatial discrete form of domain  $\Omega$  has resulted in the following global matrix form:

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & [K_T] & [G_T] \\ 0 & 0 & [K_w] \end{bmatrix} \begin{Bmatrix} U \\ T \\ p_w \end{Bmatrix} + \begin{bmatrix} [R] & [L] & [C] \\ [B_T] & [C_{TT}] & [C_{TW}] \\ [C]^T & [C_{WT}] & [C_{WP}] \end{bmatrix} \begin{Bmatrix} \dot{U} \\ \dot{T} \\ \dot{p}_w \end{Bmatrix} = \begin{Bmatrix} \dot{F} \\ F_q \\ F_w \end{Bmatrix} \quad (50)$$

#### 4.2. Integration in time

In order to discretize in time domain, the single-step integration defined in the following manner is used:

$$\int_{t_0}^{t_1} (t) dt = [(1 - \theta)u_0 + \theta u_1] \Delta t \quad (51)$$

$$\int_{t_0}^{t_1} \dot{u}(t) dt = \Delta u \quad (52)$$

where  $u_0$  and  $u_1$  are the values of the variables  $u$  at times  $t_0$  and  $t_1$ ,  $\Delta t = t_1 - t_0$  is the timestep and  $\theta$  indicates the type of interpolation;  $\theta = 0$ , forward interpolation (fully explicit),  $\theta = \frac{1}{2}$ , linear interpolation (Crank–Nicolson), and  $\theta = 1$ , backwards interpolation (fully implicit). The final matrix form is

$$\begin{bmatrix} [R] & [L] & [C] \\ [B_T] & \theta \Delta t [K_T] + [C_{TT}] & [C_{TW}] + \theta \Delta t [G_T] \\ [C]^T & [C_{WT}] & \theta \Delta t [K_W] + [C_{WP}] \end{bmatrix} \begin{Bmatrix} \Delta U \\ \Delta T \\ \Delta P_w \end{Bmatrix} \\ = \Delta t \begin{bmatrix} 0 \\ F_{q_0} - [K_T] T_0 - [G_T] p_{w_0} \\ F_{w_0} - [K_W] p_{w_0} \end{bmatrix} + \begin{Bmatrix} \Delta F_\sigma \\ \theta \Delta t \Delta F_q \\ \theta \Delta t \Delta F_w \end{Bmatrix}$$

where

$$[R] = \int_{\Omega} B^T D B d\Omega$$

$$[C] = \int_{\Omega} N^T \alpha m^T B d\Omega$$

$$[L] = \int_{\Omega} N^T \beta m^T B d\Omega$$

$$\{F_\sigma\} = \int_{\Gamma} \bar{N}^T \bar{\sigma} d\Gamma$$

$$[C]^T = - \int_{\Omega} N^T \cdot b \cdot m^T \cdot B d\Omega$$

$$[C_{wp}] = - \int_{\Omega} N_W^T \cdot C_a \cdot N_w d\Omega$$

$$[C_{wt}] = - \int_{\Omega} N_T^T \cdot C_h \cdot N d\Omega$$

$$\begin{aligned}
[K_w] &= \int_{\Omega} (\nabla N_w)^T \cdot \Lambda_w \cdot \nabla N_w \, d\Omega \\
\{F_w\} &= \int_{\Omega} (\nabla N_w)^T \Lambda_w \gamma_w \nabla z \, d\Omega + \int_{\Gamma} \bar{N}_w^T \cdot q_w \, d\Gamma \\
[K_T] &= \int_{\Omega} (\nabla N_t)^T \cdot k_t \cdot \nabla N_t \, d\Omega \\
[B_T] &= - \int_{\Omega} N^T \cdot \beta T_0 \cdot m^T [B] \, d\Omega \\
[C_{Tw}] &= - \int_{\Omega} N_t^T \cdot C_b \cdot N \, d\Omega \\
[C_{TT}] &= - \int_{\Omega} N_t^T \cdot C_T T_0 \cdot N_t \, d\Omega \\
\{F_q\} &= \int_{\Gamma} \bar{N}^T \cdot q_t \, d\Gamma
\end{aligned}$$

Based on the new model presented here, a finite element package, **STOCK**, is developed by the senior author to analyse the thermohydromechanical behaviour of repository clays in nuclear waste disposal. The conditions of stability and accuracy of the algorithm used to solve the final form matrix are investigated. It has been shown that if  $\theta$  is chosen between  $\frac{1}{2}$  and 1, the algorithm is unconditionally stable and for  $\theta < \frac{1}{2}$  the process is stable if  $\Delta t \leq 1/(\frac{1}{2} - \theta)S_n$  where  $S_n$  is the greatest eigenvalue. Accuracy conditions of numerical solution of coupled problem have been investigated by many authors like Vermeer and Verruijt,<sup>34</sup> Sandhu *et al.*,<sup>8, 35</sup> Booker and Small<sup>36</sup> and Gatmiri and Magnin.<sup>37</sup> A lower bound of timestep is given for accuracy of the solution. It depends on mechanical, hydraulic and thermal properties of material and the geometry conditions of the problem.

## 5. MECHANICAL, HYDRAULIC AND THERMAL PROPERTIES

Three types of material properties are required for the analysis of a fully coupled hydrothermo-mechanical behaviour of repository soils. In this section a brief introduction about these parameters are given.

### 5.1. Mechanical properties

In linear elastic soil model, only two parameters, Young's modulus,  $E$ , and Poisson ratio,  $\nu$ , are necessary for the description of the behaviour of soil. But in non-linear elastic (hyperbolic) model the following parameters are necessary: —  $K_L$  and  $K_u$ , loading and unloading modulus number;  $K_b$ , bulk modulus number,  $n$ ,  $R_f$  and  $m$ , constants (all dimensionless),  $p_{atm}$ , atmospheric pressure, and  $\sigma_1, \sigma_3$ , principal stresses. It is obvious that the above parameters are defined from the Laboratory tests in practice and they are the necessary data to carry out the calculation. The parameters of hyperbolic model can be defined in other manners. Having the initial stress state,

the terms of elasticity (linear) matrix can be known. Once this matrix is known, the final stiffness matrix in the different stress or strain levels can be calculated. This procedure should be repeated at each iteration step.

As it is described in Section 3, the thermal-hyperbolic model presented here, can incorporate the effect of temperature on the tangent modulus by using equation (38). A parameter  $m_1$  (constant) is added to model. The bulk modulus is calculated from the state surface of void ratio. In such a manner the effects of stress and temperature are included in the model. Thus, two parameters of Kondner–Duncan model can be reduced ( $K_b, m$ ), but, in order to define the thermal state surface of void ratio the following parameters are added:  $C_{cv}$ , isothermal compressibility index in  $(e - \lg p')$  co-ordinates;  $\alpha_0, \alpha_1, \alpha_2$  and  $\alpha_3$ , constants ( $1/^\circ\text{C}$ ).

Some information about the above parameters for Boom clay and Pontida silty clay can be found in Reference 38.  $C_{cv}$  is a known parameter similar to  $\kappa$  in critical state theory in isothermal conditions. Biot hydromechanical coupling coefficient  $\alpha$  in the water-saturated soil can be evaluated near 1 without any significant error, but for rock mass and the other saturating fluid, it should be evaluated correctly.

The other mechanical parameters of materials are  $1/K_s$  and  $1/K_w$ , compressibility of solid grains and fluid. They are very well-known for soil particles and water.

## 5.2. Thermal properties

The thermal parameters considered in the development of the equations are:  $\alpha_s, \alpha_w, C_s, C_w$  which are involved in the following terms:

$$C_h = (\alpha - n)\alpha_s + n\alpha_w$$

$$C_b = (\rho c)_M - \{(1 - n)C_s\rho_s\alpha_s + nC_w\rho_w\alpha_w\}T_0$$

where  $(\rho c)_M = (1 - n)C_s\rho_s + nC_w\rho_w$  is the solid–fluid heat capacity. The solid and fluid thermal conductivities ( $k^s$  and  $k^w$ ) are the two other parameters used in this analysis.  $\beta$ , the thermo-mechanic coupling coefficient is not an independent parameter of the above six properties. The relationship can be expressed through the equation

$$\beta = (2G + 3\lambda)\alpha_s = 3K'\alpha_s.$$

$\beta$  is usually negative, and the increase in temperature leads to a volumetric expansion. In this definition of  $\beta$ , the thermal volume of expansion of soil mixture due to physicochemical effects is neglected. From the given classical expression of  $\beta$  (above equation), it can be observed that, in non-linear model  $\beta$  depends on effective stress and temperature. This dependency has been observed in experiments on the normally, lightly or highly overconsolidated clay but the available data are insufficient to determine the exact dependency. The method used in this approach can be considered as an attempt to model these effects. The coefficient of volume expansion of soil particles,  $\alpha_s$ , is considered constant which appears logical. The direct measurements of  $\alpha_s$  are not available. For Boom clay, Pontida clay, illite and kaolinite the values given by Hueckel and Pellegrini,<sup>38</sup> and Campanella and Mitchell<sup>39</sup> can be used. The coefficient of volume expansion of pore water  $\alpha_w$  is considered constant in this study because of the lack of experimental evidence available in the literature. Generally,  $\alpha_w$  is sensitive to temperature change and insensitive to variation of pore water pressure. Chapman<sup>40</sup> has given the variation of coefficient of thermal

volume expansion of pore water with temperature reported by Seneviratne *et al.*<sup>41,42</sup> Baldi *et al.*<sup>43</sup> have studied the effects of pore water pressure and temperature on the coefficient of thermal volume expansion of water; based on reported data the following approximate formula for  $\alpha_w$  is proposed:

$$\alpha_w(T, p) = \alpha_0 + (\alpha_1 + \beta_1 T) \ln(mp) + (\alpha_2 + \beta_2 T) (\ln(mp))^2$$

the constants  $\alpha_0, \alpha_1, \alpha_2, \beta_1, \beta_2$  and  $m$  have been given in Reference.<sup>43</sup>

### 5.3. Hydraulic properties

The principal hydraulic parameter is permeability of solid skeleton. The effect of temperature on the permeability is introduced by change of viscosity due to temperature variations. A formula has been derived by fitting the experiment values given in Table I.

The effect of volume change of skeleton on the permeability is introduced via void ratio or porosity. The current permeability can be related to the reference permeability,  $\Lambda_{w0}$ , by the third power of porosity ratios in the current and reference states. Therefore, the following equation can present the temperature and stress level effects on permeability:

$$\Lambda_w = \Lambda_{w0} \frac{v_i}{v} \left( \frac{e}{e_i} \right)^3$$

## 6. APPLICATION, VALIDATION AND COMPARATIVE ANALYSES

The presented formulation encoded in a particular purpose finite element program has been used to calculate the results for the test and application cases given.

### 6.1. One-dimensional transient heat flow in dry soil

A layer of elastic soil of thickness  $h$  is under uniform absolute temperature  $T_0$  throughout the initial form. The mesh and the boundary conditions used for this one-dimensional problem is given in Figure 2(a). A temperature increase ( $\theta_0$ ) is imposed at the unstressed surface. The results of temperature distribution within the depth at different times (temperature isochrone) are calculated numerically as well as analytically using the exact solution given in Reference 44 as

$$\bar{\theta} = \frac{\theta_0 \cosh(\mu z)}{s \cosh(\mu h)} \quad \text{and} \quad \bar{w} = \left( \frac{\theta_0}{\mu s} \right) \left( \frac{\beta}{M} \right) \frac{\cosh(\mu z)}{\cosh(\mu h)}, \quad \mu = \sqrt{\frac{sA}{kM}}$$

where  $\bar{\theta}$  and  $\bar{w}$  are the Laplace transform of the temperature change and vertical displacement, respectively,  $k$  is thermal diffusivity, and  $s$  is the Laplace transform variable.  $A$  and  $M$  are the constrained moduli for adiabatic and isothermal conditions.  $M$  is the modulus which, in soil

Table I. Values of dynamic viscosity as a function of temperature

$T$	0	10	20	40	60		°C
$v$	$1.78 \times 10^{-6}$	$1.3 \times 10^{-6}$	$1.0 \times 10^{-6}$	$0.67 \times 10^{-6}$	$0.48 \times 10^{-6}$	$0.36 \times 10^{-6}$	$\text{m}^2/\text{s}$

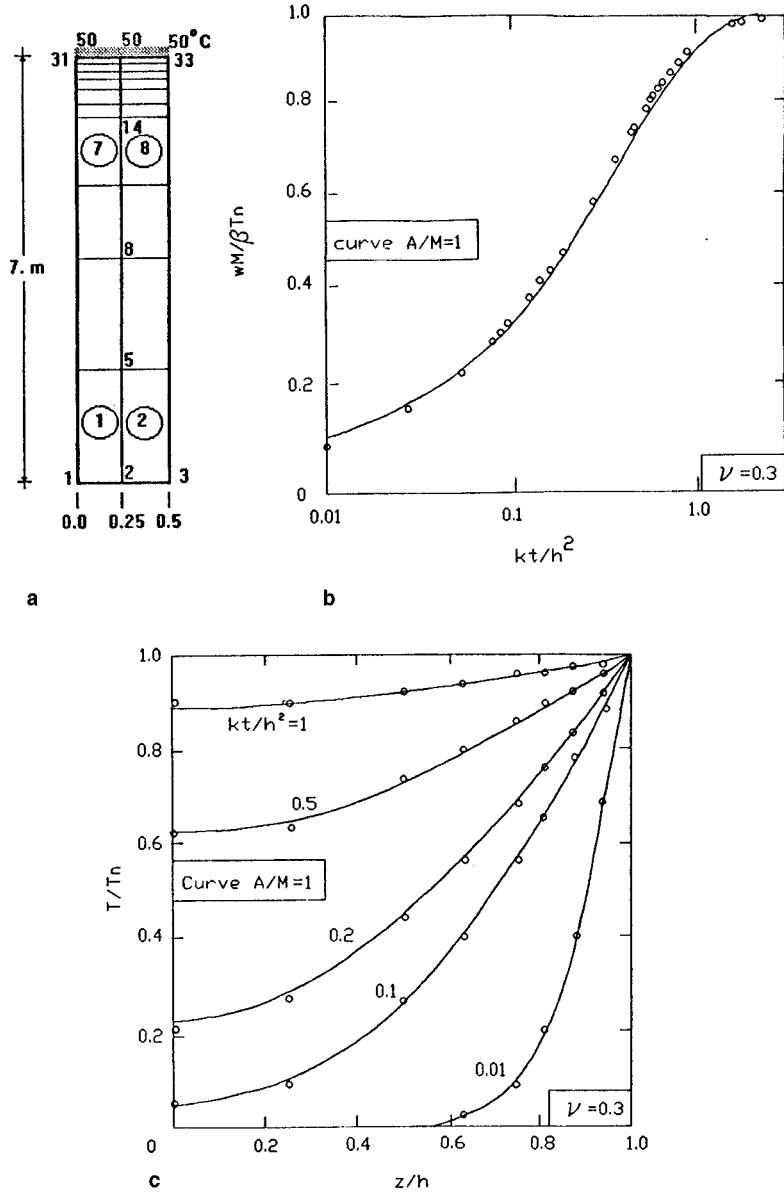


Figure 2. Result of dry column test: (a) used mesh; (b) surface heave; (c) temperature isochrones

mechanics, is well known as  $\lambda + 2G$  with the Lamé constants and  $A$  is given by

$$A = (\lambda + 2G) + \beta^2 T_0 / m \beta$$

is thermoelastic coupling coefficient and  $m$  is the specific heat for total mass at constant volume or heat capacity which is  $(1 - n)\rho_s C_s$  in our formulation. The dimension of elastic and thermal properties are the following:  $\beta$ ; Pa/°C or N/m²/°C;  $m$ , J/m³/°C;  $k$ , m²/s;  $M$ , A; Pa or N/m².

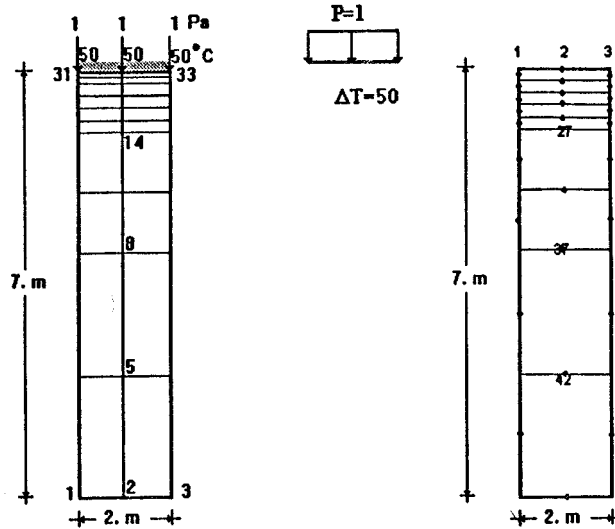


Figure 3. One-dimensional thermoelastic model

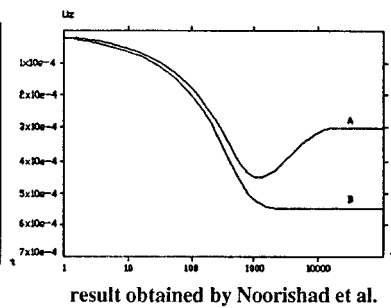
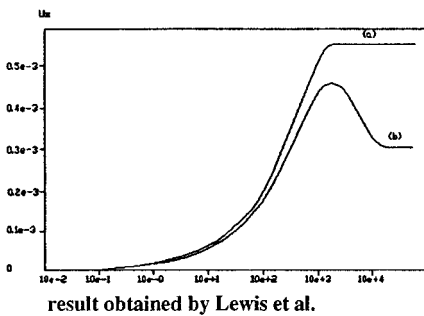
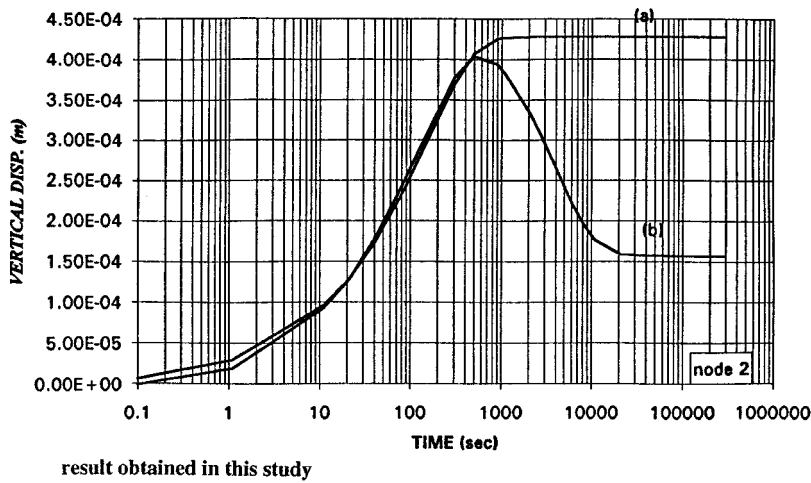


Figure 4. Comparison of surface settlement and heave

The case  $M = A$  corresponds to simply one-dimensional heat diffusion. The comparisons between numerical and analytical results for  $A = M$  are presented in Figure 2. This figure presents the surface heave (2(b)) and the temperature isochrones (2(c)) at different times. The accuracy of the finite element formulation and encoding is validated by very satisfactory agreement between the analytical and numerical solutions.

6.2. Thermoelastic consolidation in saturated soil

Aboustit *et al.*<sup>24,25</sup> have given the non-convective coupled finite element formulation of quasi-static thermoelastic consolidation in the frame of linear elastic behaviour by assuming the infinitesimal strain and an incompressible fluid flow in this porous medium. The sand column considered by Aboustit *et al.* and the mesh used for numerical calculation and boundary conditions are presented in Figure 3. The parameters used in this analysis are: Young's modulus  $E = 6000 \text{ Pa}$ ; Poisson ratio  $\nu = 0.4$ ; hydraulic permeability  $\Lambda = 4E-6 \text{ m/s}$ ; Biot hydromechanic

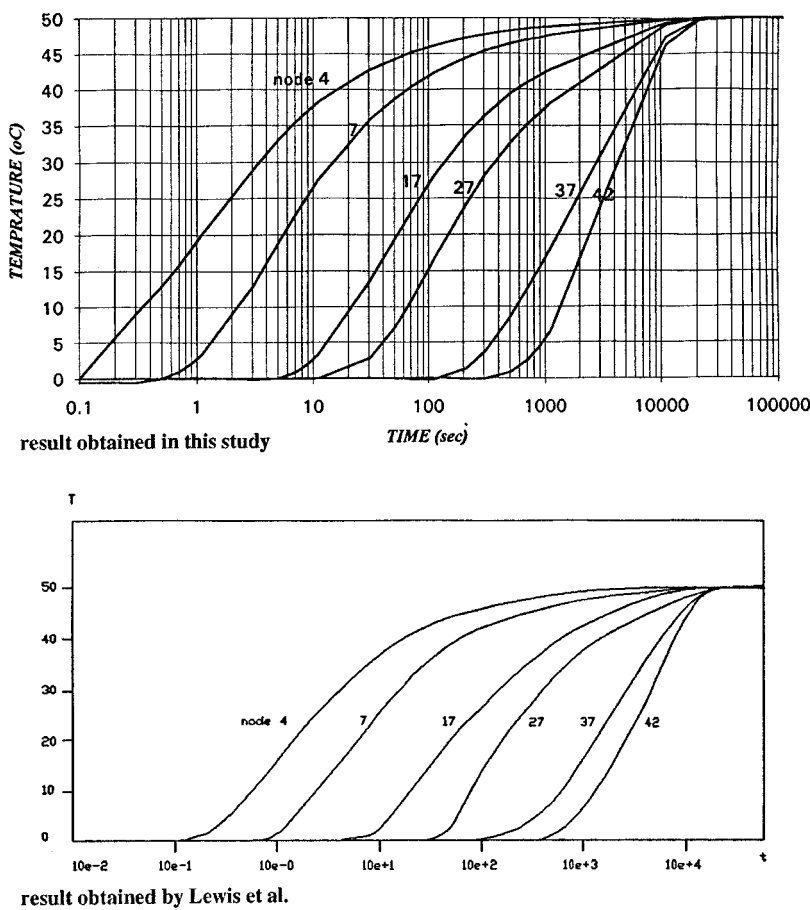


Figure 5. Temperature versus time at different nodes



coupling coefficient  $\alpha = 1$ ; thermal conductivity,  $k = 0.2 \text{ cal/m/s/}^\circ\text{C}$ ; heat capacity of matrix  $(\rho C)_M = 40 \text{ kcal/m}^3/^\circ\text{C}$  and thermal expansion coefficient  $\beta = 0.3 \times 10^{-6} \text{ 1/}^\circ\text{C}$ .

The presented approach in this study is not exactly the same with the approach given by Aboustit *et al.*<sup>24,25</sup> The contributions of the matrix terms which are zero in the approach of Aboustit *et al.*<sup>25</sup> can be a source of very small differences which will be observed during the comparison. In fact, we have tried to have very small terms in the matrix in the place of zero terms in Aboustit *et al.*

Figure 4 presents a comparison between surface settlement of the saturated column considered by Aboustit *et al.* in isothermal and non-isothermal cases given by Lewis *et al.*<sup>28</sup>, and Noorishad *et al.*<sup>20</sup> and this study. In this example the water viscosity, thermal expansivity variations and fluid incompressibility are considered.

In Figure 5, the evolution of temperature in time for some nodal points are plotted and compared with the results presented by Lewis *et al.*<sup>28</sup> Displacement versus time at different nodes

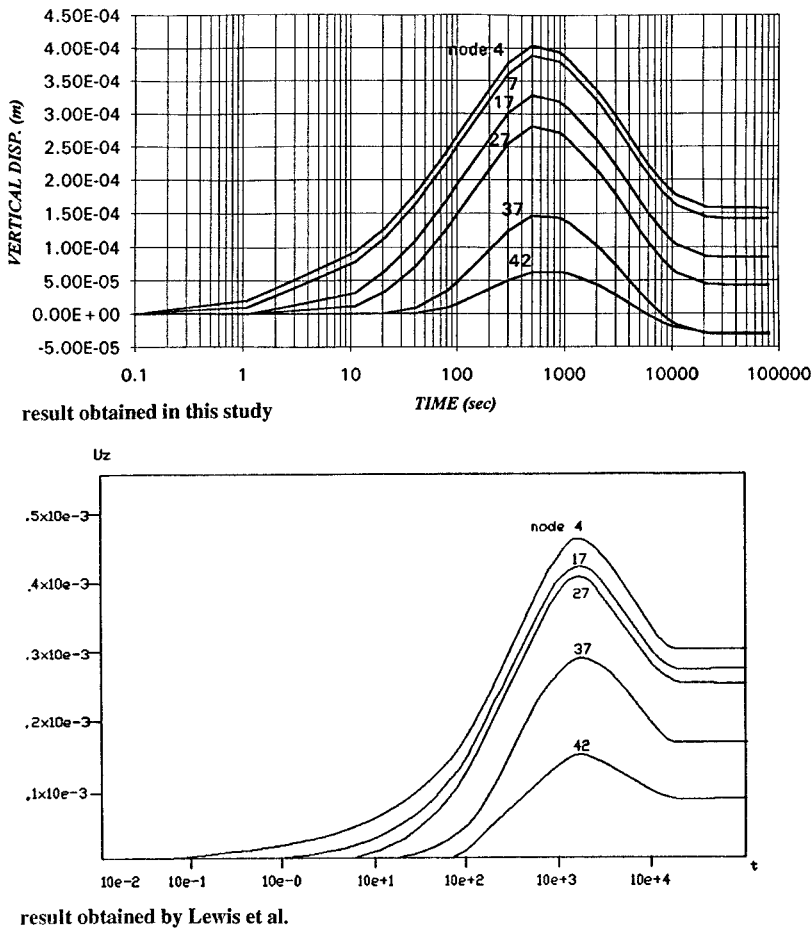
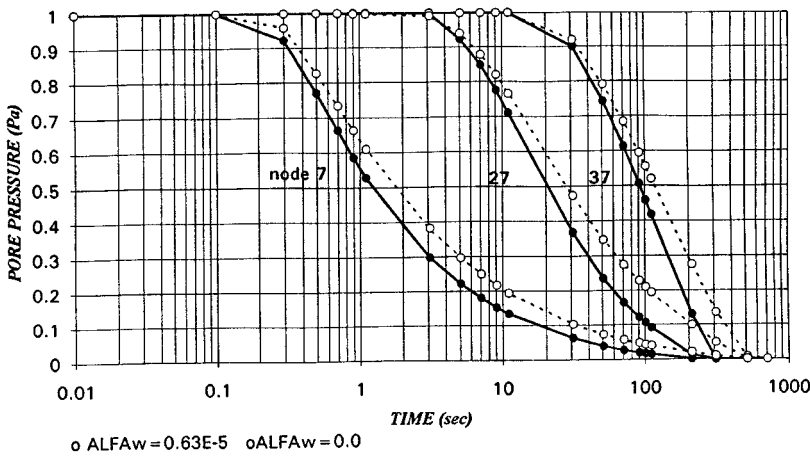


Figure 6. Displacement versus time at different nodes

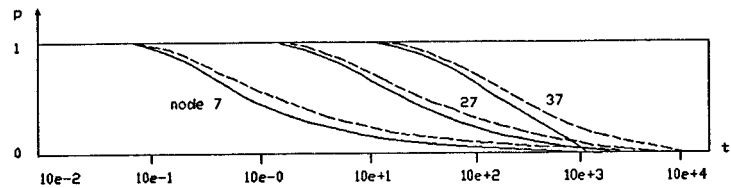
are given in Figure 6. In the first steps the compressibility of the skeleton is more significant. After a necessary time for temperature distribution, which is not small, the reversal tendency of displacement can be observed. The temperature increase is very slow and the expansion due to thermal effects are effective after this time. Pore pressure variations for some nodes in time are presented in Figure 7 and compared with the results obtained by Lewis *et al.*<sup>28</sup> In this figure two different cases are presented: one case in which the thermal expansion coefficient of water is considered to be equal to  $0.63 \times 10^{-5}$  and the other case with this coefficient equal to zero. The isochrones of pore pressures and temperatures are given and compared with that obtained by Aboustit *et al.*<sup>24,25</sup> in Figure 8.

6.3. Non-linear elastic model

The same saturated column is considered, but in order to investigate the non-linearity effect the following parameters for hyperbolic model are used:  $K_L = K_u = 60$ ;  $n = 0.5$ ;  $R_f = 0.75$ ;  $K_b = 100$ ;  $m = 0.2$ . The values of the elastic and bulk moduli with time are shown in Figure 9. The hardening effect of stress level can be observed. This hardening effect is combined with softening effect of temperature during the evolution of pore pressure and temperature. With the set of mechanical



result obtained in this study



result obtained by Lewis et al.

Figure 7. Pore pressure versus time at different nodes

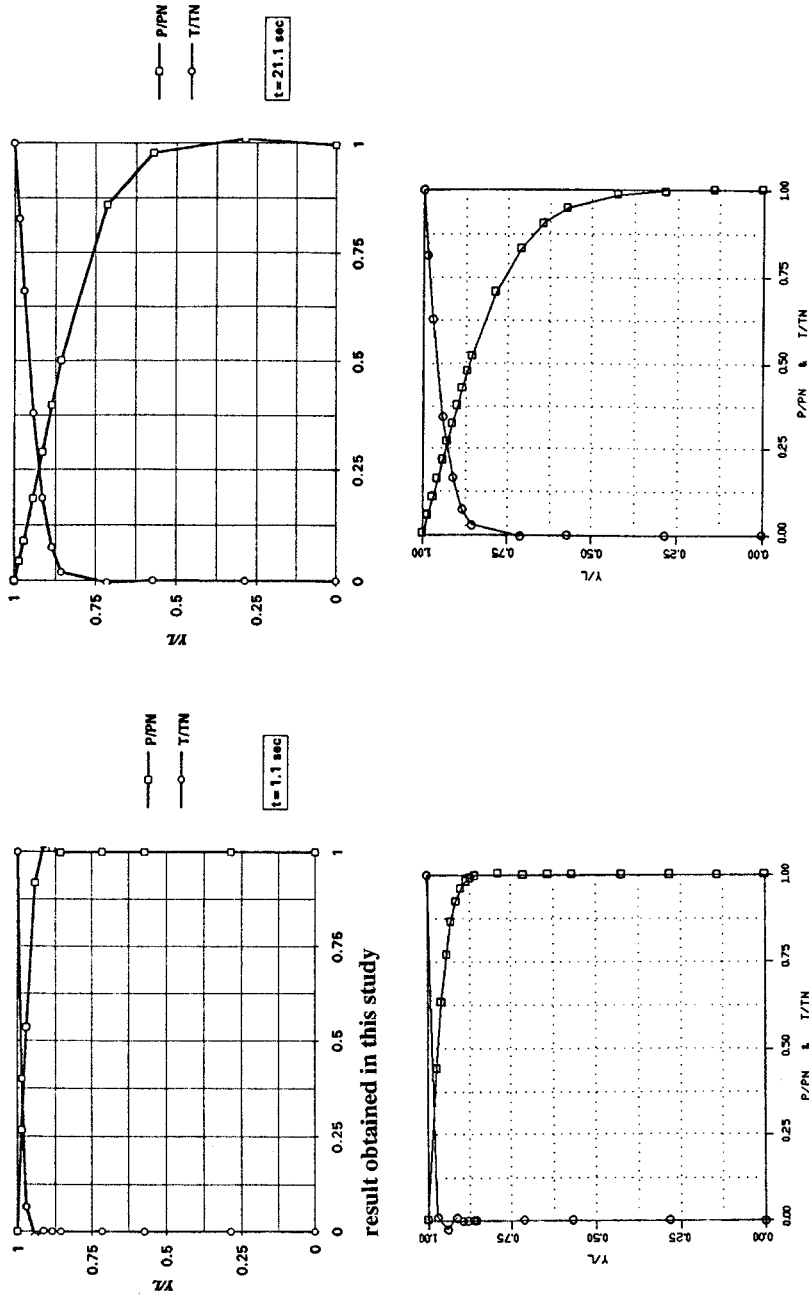


Figure 8. Pore pressure and temperature profiles at different times

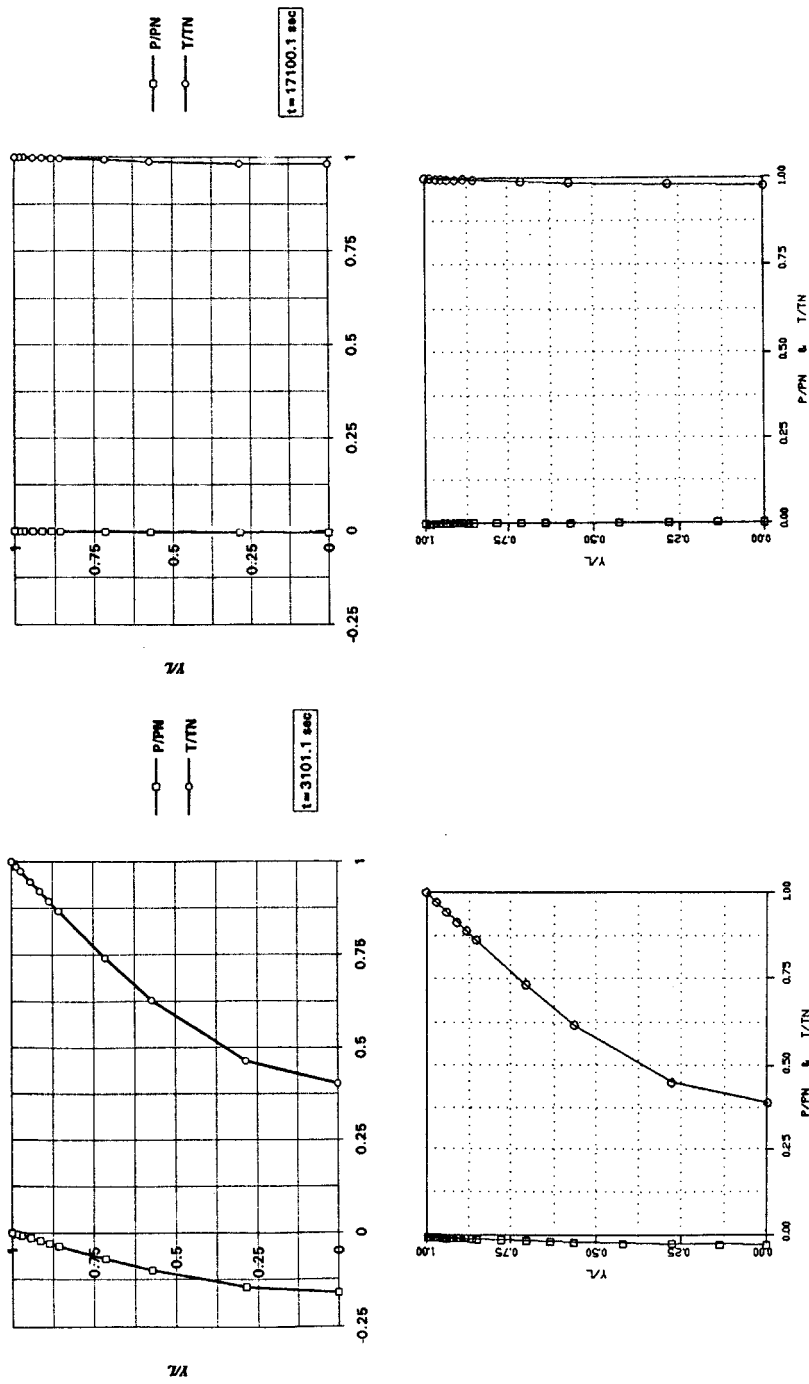


Figure 8. Continued

and thermal parameters chosen in this example, the hardening effect is predominant. The real parameters of a soil may lead to predominant thermal softening effect or stress hardening effects.

Figure 10 shows the comparison between settlements at different nodes obtained by linear elastic and non-linear elastic model. Figures 11 and 12 present the evolution of temperature and water pore pressure in linear elastic and non-linear elastic models, respectively. Isothermal and non-isothermal surface settlements obtained in the frame of hyperbolic model and linear elastic behaviour are presented in Figure 13.

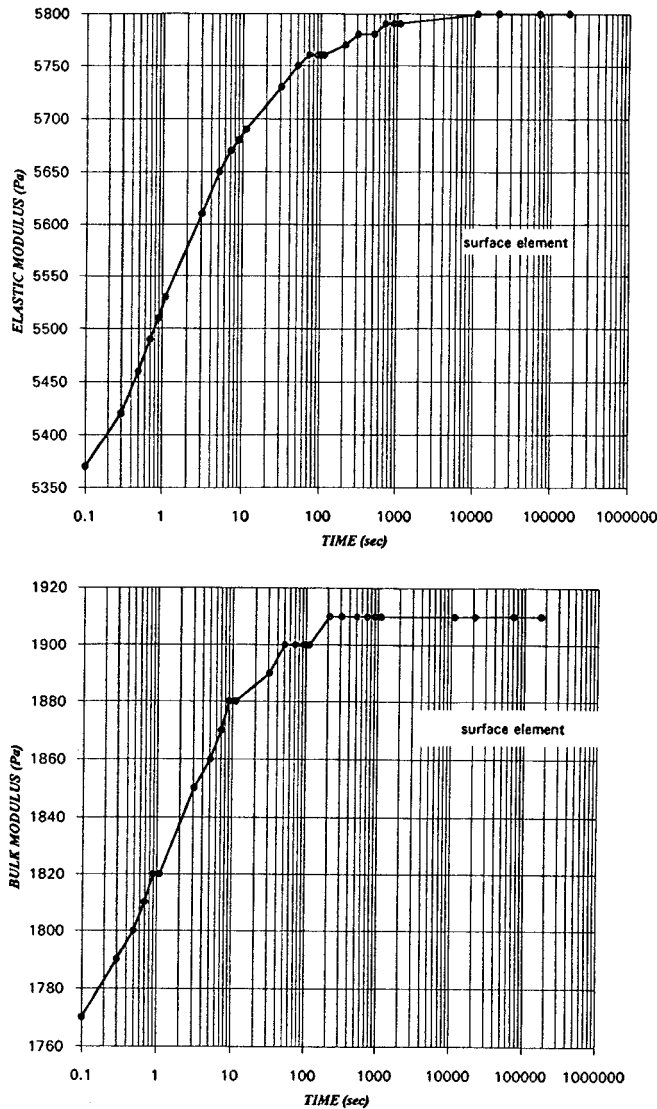


Figure 9. Variation of elastic and bulk moduli with time

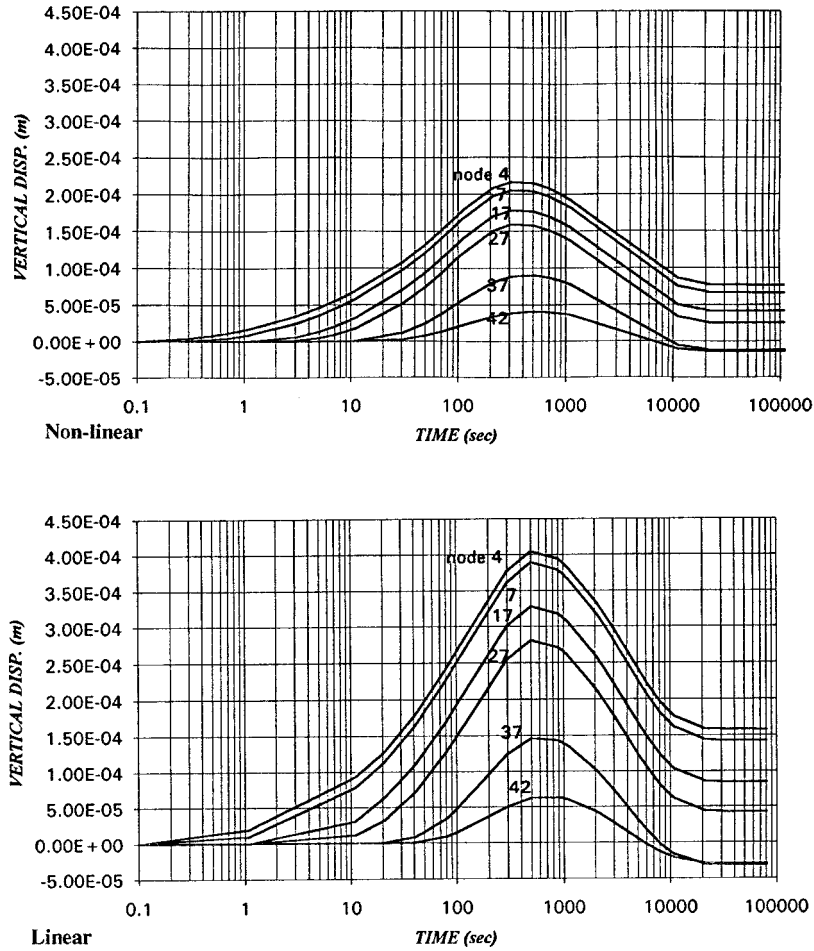
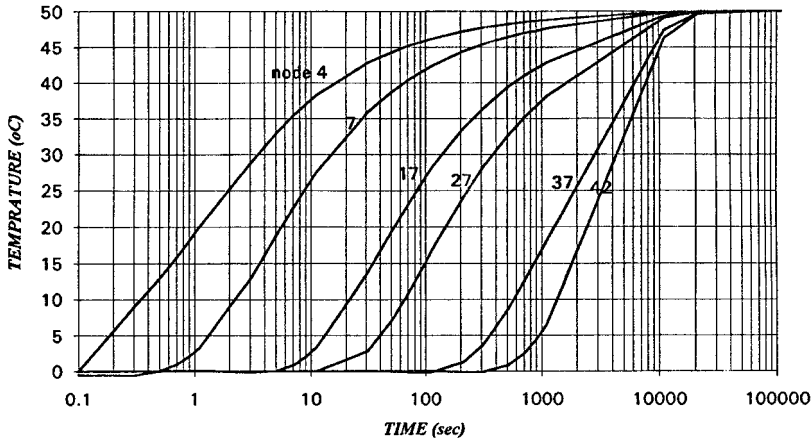


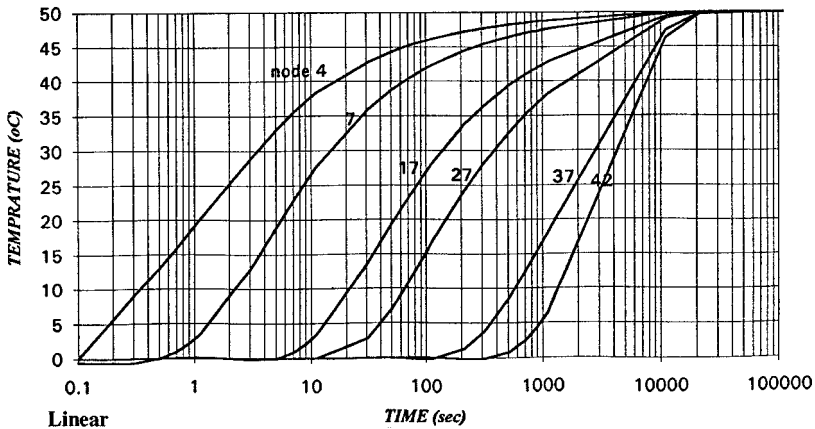
Figure 10. Comparison of settlements in linear and non-linear elastic models

# 7. CONCLUSION

The main objective of this study was to prepare a finite element code for analysing the effect of temperature variations in a saturated porous media such as clays which are the repository soils in nuclear waste disposal. A new finite element model for fully coupled thermohydromechanical behaviour of saturated clays was developed. In this model, a new concept called 'thermal void ratio state surface' has been introduced. The basic equations for solid skeleton, fluid phase and thermal energy transfer are derived in a general form. Minimum of simplifying assumptions are taken into account. The convective terms, present in the formulation, are not included in the computer code as it can be done easily. The model considers the effect of temperature changes on the mechanical properties such as Young modulus and bulk modulus, as well as on the



Non-linear



Linear

Figure 11. Comparison of temperature in linear and non-linear elastic models

hydraulic properties such as permeability and thermal parameters used in the present formulation. Non-linear (hyperbolic) constitutive law is used and the effect of stress level on the mentioned properties are assumed. The finite element model was developed for both drained and saturated cases. Several comparisons are made in order to validate the model and finite element code. The analytical thermoelastic solution is compared with the results of this model. Code-to-code comparisons are carried out for drained (dry) thermoelastic one-dimensional and linear thermohydroelastic consolidation in one and two-dimensional cases. The obtained results validated the prepared finite element code. An example of non-linear thermohydroelastic consolidation of a saturated column by using the new concept, thermal void ratio state surface which reflects the effects of temperature softening in a non-linear behaviour, is carried out and differences between the results obtained by this new model and those obtained by the classical

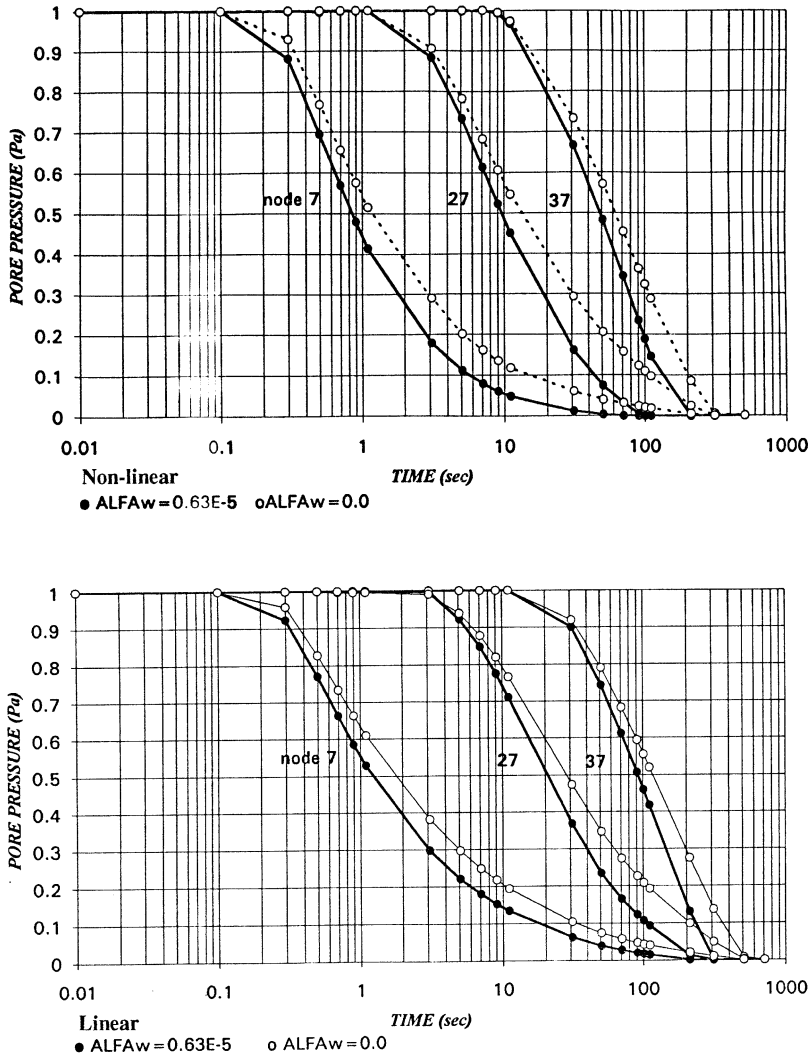


Figure 12. Comparison of pressure in linear and non-linear elastic models

elastic models are discussed. From this study the following points can be concluded:

- The thermal void ratio state surface can be efficient to estimate the bulk modulus,
- The non-linear thermohydromechanical model is more useful and near to real behaviour of soil under thermal and mechanical loading,
- stress-induced hardening and temperature-induced softening and their combined effect is well considered in thermal non-linear behaviour presented in this model, and
- the effects of stress and temperature changes on the thermal and hydraulic properties of soil are considered in this study.



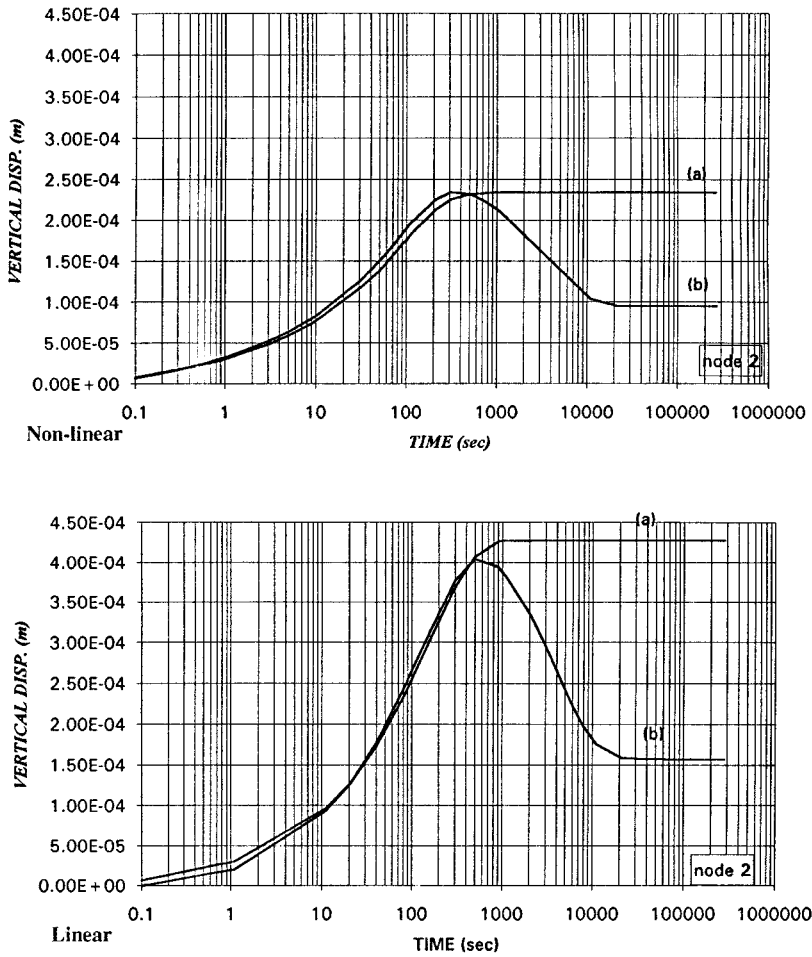


Figure 13. Comparison of surface settlements in linear and non-linear elastic models

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